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Electromagnetic Wave Scattering by the Edge of a Carbon Nanotube

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Abstract

Scattering of a time–harmonic electromagnetic field by the edge of a semi–infinite, single–wall, zigzag carbon nanotube (CN) is considered. The Wiener–Hopf technique is applied to determine the exact solution of the problem, and the scattering pattern is numerically calculated in the vicinity of the main plasmon resonance frequency.

1. Introduction

Since the discovery by Iijima of quasi–one–dimensional cylindrical crystalline structures of carbon atoms, generally referred to as carbon nanotubes (CNs), many unique physical properties of theirs have been predicted theoretically and detected experimentally [1]. In particular, with reference to their optical properties, thin films comprising aligned CNs have been described theoretically as composite mediums [3, 4].

A composite medium consists of a homogeneous host medium with periodically or randomly dispersed inclusions. The inclusions must be electrically small for *local* homogenization to be possible, for which purpose each inclusion is represented by a polarizability tensor [5]. Furthermore, macroscopic samples of a composite medium are supposed to contain a huge number of inclusions, so that the composite medium can be replaced by an effectively homogeneous medium.

The polarizability tensor of a single CN in isolation has been treated approximately by several researchers. For instance, the 3–D polarizability tensor of a *zigzag* CN was calculated by Ma & Yang [6] when its length L and cross–sectional radius R are small compared to the free–space wavelength $\lambda = 2\pi/k$ (i.e., $kL \ll 1$ and $kR \ll 1$). The 2–D polarizability tensor (per unit length) of infinitely long CNs has also been treated [3, 4, 7]. However, in the optical frequency range, the typical geometric parameters of actual CNs satisfy the following conditions:

$$kR \ll 1, \quad L \gg R, \quad kL \sim 1. \tag{1}$$

Such conditions are characteristic of wire antennas at microwave frequencies [8]. A wire antenna cannot be characterized by a polarizability tensor, because the contribution of the

high–order multipoles to the scattered field is strong due to the last condition in Eqs. (1). Scattering by a long wire is much too complicated to be expressed *via* a dipole, and arrays of many long wires can not therefore be homogenized in the same way as arrays of electrically small inclusions can be [5]. The essential quantity required is the scattering matrix (or its equivalent) of a single wire [9]. From this quantity, the scattering pattern of a wire array can be calculated [10]. Analogously, the key problem for the optical response of CN arrays in the optical regime defined by Eqs. (1) is the calculation of the scattering pattern of an isolated CN of finite length. Of course, care must be exercised because CNs can not be necessarily assumed as perfect conductors — unlike wire antennas.

The effective boundary conditions for a CN are non–trivial [11]. Accordingly, the responses of CNs are different from those of wire antennas. For example, strongly attenuated surface polaritons [11] and plasmons [2] appear in CNs, instead of the weakly attenuated waves of longitudinal current in wire antennas. Yet the universality of macroscopic electrodynamics means that certain common effects are possible. In particular, we expect resonance effects, which can arise as a result of the interactions between the edges of a CN.

This paper addresses the electromagnetic scattering properties of CNs. We use the Wiener–Hopf technique [12] and the effective impedance boundary conditions [11] for a semi–infinite, single–shell, zigzag CN. The scattering amplitude of a finite–length CN can be expressed in terms of the scattering response of a semi–infinite CN, using the edge–wave method.

2. Theoretical Framework

Consider a CN aligned parallel to the z axis of a circular cylindrical coordinate system (r, ϕ, z) whose origin is located at the center of the circular cross–section of the CN. The edge of the CN can be either closed or open. If closed, the edge is almost hemispherical. However, the oxidation of CNs makes the open–edge configuration more probable — which is fortuitous, as that configuration is the more suitable of the two for theoretical analysis. But the scattered field is almost independent of the edge configuration if the first of Eqs. (1) holds true, in direct analogy with hollow and dense wire antennas [12]. Hence, we restrict ourselves to the open–edge configuration.

Let the incident field be E–polarized, with harmonic time–dependence of $e^{-i\omega t}$, and propagating at an angle θ_0 with respect to the z axis. This field is represented by the Hertz potential $\psi^{(i)}$. The total potential $\psi_\Sigma = \psi^{(i)} + \psi^{(s)}$, where $\psi^{(s)}$ corresponds to the scattered field as per

$$\mathbf{E}^{(s)} = -\frac{1}{ik}\frac{\partial^2\psi^{(s)}}{\partial z \partial r}\mathbf{u}_r + \frac{1}{ikr}\frac{\partial^2\psi^{(s)}}{\partial z \partial \phi}\mathbf{u}_\phi - \frac{1}{ik}\left(\frac{\partial^2\psi^{(s)}}{\partial z^2} + k^2\psi^{(s)}\right)\mathbf{u}_z\,, \tag{2}$$

$$\mathbf{H}^{(s)} = \frac{1}{r}\frac{\partial\psi^{(s)}}{\partial\phi}\mathbf{u}_r - \frac{\partial\psi^{(s)}}{\partial r}\mathbf{u}_\phi\,. \tag{3}$$

The boundary conditions satisfied are as follows (in Gaussian units) [11]:

$$\left.\begin{array}{l} \left(1 + \frac{\tilde{l}_0}{k^2}\frac{\partial^2}{\partial z^2}\right)\left(\left.\dfrac{\partial\psi^{(s)}}{\partial r}\right|_{r=R+0} - \left.\dfrac{\partial\psi^{(s)}}{\partial r}\right|_{r=R-0}\right) = \frac{4\pi\tilde{\sigma}_{zz}}{i\omega}\left(\dfrac{\partial^2\psi^{(s)}}{\partial z^2} + k^2\psi^{(s)}\right) + \Phi(\phi, z)\,, \\ \hfill 0 < z < \infty\,, \\ \left.\dfrac{\partial\psi^{(s)}}{\partial r}\right|_{r=R-0} = \left.\dfrac{\partial\psi^{(s)}}{\partial r}\right|_{r=R+0}\,, \qquad \psi^{(s)}|_{r=R+0} = \psi^{(s)}|_{r=R-0}\,, \qquad -\infty < z < \infty \end{array}\right\}\,, \tag{4}$$

Here, $\Phi(\phi, z) = \frac{4\pi}{c}k\tilde{\sigma}_{zz}\,\psi^{(i)}(R, \phi, z)\,\sin^2\theta_0$ emerges from the incident field; c is the speed of light in vacuum; the parameter $\tilde{l}_0$ takes spatial dispersion into account [11]; and $\tilde{\sigma}_{zz}$ is the axial

conductivity of an isolated CN. Both $\tilde{\sigma}_{zz}$ and $\tilde{l}_0$ have been calculated *via* quantum transport theory [11]. The boundary conditions (4) have to be complemented by radiation conditions as well as by edge conditions [12].

The boundary value problem may be solved with the Wiener–Hopf technique, with the Jones method employed to derive Wiener–Hopf functional equation:

$$\mathcal{J}_+(\alpha)G(\alpha) = \Psi_-(\alpha) - \frac{\breve{\Phi}(\phi,\alpha)}{\xi\gamma^2}. \tag{5}$$

Here, $\breve{\Phi}(\phi,\alpha)$ is the spatial 1-D Fourier transform of $\Phi(\phi,z)$ with α as the (complex-valued) spatial frequency corresponding to z; $K_l(\cdot)$ and $I_l(\cdot)$ are modified Bessel functions of order $l \geq 0$; $G(\alpha) = K_l(\gamma R)I_l(\gamma R)R - \Gamma\xi^{-1}\gamma^{-2}$, $\xi = -4i\pi\tilde{\sigma}_{zz}/\omega$, $\Gamma = 1 - \tilde{l}_0\alpha^2k^{-2}$ and $\gamma = \sqrt{\alpha^2 - k^2}$; while $\mathcal{J}_+(\alpha)$ and $\Psi_-(\alpha)$ are two unknown functions to be determined as per the Wiener–Hopf technique. In order to solve Eq. (5) analytically, one has to apply the usual factorization and decomposition procedures, and the exact analytical expression for the scattered Hertz potential is then obtained by the inverse spatial Fourier transform.

In the far zone, application of the saddle point method leads to

$$H_\phi^{(s)},\, E_\theta^{(s)} \sim F_l(\theta,\theta_0)\,\frac{e^{ik\sqrt{r^2+z^2}}}{k\sqrt{r^2+z^2}}, \tag{6}$$

where $\theta = \pi - \tan^{-1}(r/z)$ and

$$F_l(\theta,\theta_0) = \frac{H_l^{(1)}(kR\sin\theta_0)}{G_+(k\cos\theta_0)(1+\cos\theta_0)} \times \frac{\cos(\theta/2)}{\sin(\theta/2)} \times \frac{J_l(kR\sin\theta)e^{-i\pi/4}}{(\cos\theta+\cos\theta_0)\; G_-(k\cos\theta)}; \tag{7}$$

$H_l^{(1)}(\cdot)$ is the cylindrical Hankel function and $J_l(\cdot)$ the cylindrical Bessel function of order l; while $G(\alpha) = G_+(\alpha)G_-(\alpha)$. The function $F_l(\theta,\theta_0)$ is the *scattering pattern* of the edge. The full scattering pattern of a CN includes additional components accounting for surface polaritons.

3. Numerical Results and Discussion

We calculated the far–zone scattered power density $P(\theta) \sim |F_0(\theta,\theta_0)|^2$, with $l = 0$ sufficing for most realistic incident fields. Following Ref. [11], we set the inverse relaxation time $\nu = 0.33 \times 10^{12}\ \mathrm{s}^{-1}$, which is in good agreement with the recent measurements of dynamic room–temperature conductivity of mats of single–wall CNs [13].

Let us examine $P(\theta)$ in the vicinity of $\beta = 1$, where $\beta = \hbar\omega/2\gamma_0 = 1$, $\hbar$ is the Planck constant, and γ_0 is the so–called overlap integral [11]. This case is of special interest since it corresponds to the main plasmon condition [2] for all types of CNs. All other resonant lines are interpreted as its satellites. Sample plots of $P(\theta)$ calculated in the regime $0 < \theta < \pi - \theta_0$ are presented in Figure 1. Let us point out here that the saddle point method is inapplicable in the vicinity of $\theta = \pi - \theta_0$.

It is clear from Figure 1 that a relatively weak deviation from the exact resonance condition $\beta = 1$ leads to a significant decrease in the scattered field intensity; and we deduce thereby that scattering by a semi–infinite CN is essentially due to plasmon propagation. We also infer from Figure 1 that *forward scattering* is stronger by 2 to 3 orders in magnitude than *backscattering*. This effect persists for all types of CNs in a wide frequency range.

To conclude, we have investigated the scattering of a time–harmonic electromagnetic field by a semi–infinite, single–shell, zigzag CN. We have found an exact analytical solution in the framework of the Wiener–Hopf technique. The solution found will serve as the basis of the theory of light scattering by single CNs and CN–based composites.

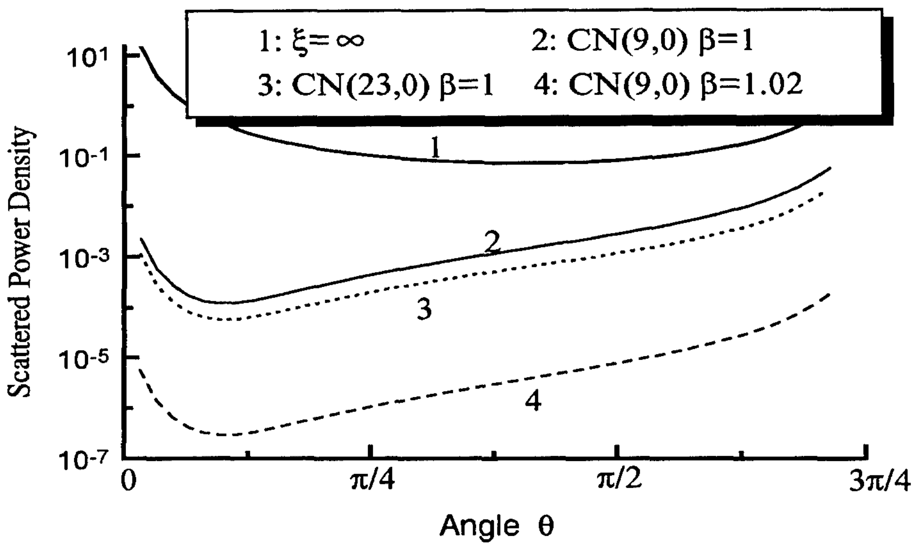

Figure 1: Sample plots of the scattered power density $P(\theta)$ for semi–infinite, single–shell, zizgag CNs (m, $n = 0$), when $\theta_0 = \pi/4$. For comparison, the results for $\xi = \infty$ (i.e., perfect conduction) are also shown.

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